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TUBULAR CHEMICAL REACTORS: THE "LUMPING APPROXIMATION" AND BIFURCATION OF OSCILLATORY STATES*

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Abstract. We study axial heat and mass transfer in a highly diffusive tubular chemical reactor in which a simple reaction is occurring. Singular perturbation techniques are used to derive approximate equations governing the situation. Attention is then focused on the bifurcation of oscillatory states from steady operating characteristics. By means of numerical calculations and phase plane illustrations we follow the bifurcated periodic solution branches along their complete lengths.

1. Introduction. The mathematical problem of axial heat and mass transfer in a chemical tubular reactor in which a simple reaction is occurring is described by a set of nonlinear parabolic partial differential equations which in dimensionless form can be written as (see Hlavacek and Hofmann [4])

$$
\begin{aligned}
&T_t = (1/P)T_{xx} - T_x - \beta(T - T_c) + DBf(T, C),\\
&C_t = (1/P)C_{xx} - C_x + Df(T, C),\\
&T_x(0, t) - PT(0, t) = 0,\\
&C_x(0, t) - PC(0, t) = 0,\\
&T_x(1, t) = 0,\\
&C_x(1, t) = 0,\\
&T(x, 0) = \phi(\kappa),\\
&C(x, 0) = \psi(x).
\end{aligned}
\tag{1.1}
$$

The nonlinearity $f(T, C)$, the rate function, is given by

$$f(T, C) = (1 - C)\, e^{T/(1+\varepsilon T)}.$$

T_c, P, β, D and ε are nonnegative constants. C is the conversion or product concentration of a chemical whose temperature is T.

For the case $\beta = 0$ (the adiabatic reactor) the investigation of the time-dependent solutions of (1.1) reduces to a study of

$$
\begin{aligned}
(1/P)T'' - T' - D(B - T)\, e^{T/(1+\varepsilon T)} &= 0,\\
T'(0) - PT(0) &= 0,\\
T'(1) &= 0,
\end{aligned}
\tag{1.2}
$$

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where the concentration C is given by T/B. The questions of multiplicity and stability for (1.2) were studied by Cohen [1].

For $\beta > 0$ (the nonadiabatic reactor) the problem (1.1) has been investigated numerically by McGowin and Perlmutter [7], Hlavacek and Hofmann [4], [5], and Hlavacek, Hofmann and Kubicek [6]. For various values of the parameters T_c, P, β, D and ε the existence of one, three and five steady states and the existence of oscillatory solutions are reported. Due to the large number of parameters and the great variation in their possible numerical values, an exhaustive treatment of the problem has yet to be given. One of the results of the present paper will be that for $0 < P \ll 1$ and any allowed values of the other parameters we shall account for all possible phenomena which can occur in (1.1).

Our investigation of the problem (1.1) will be for the case $0 < P \ll 1$ which means physically that the diffusion coefficients are large. By the formal methods of singular perturbation theory we shall show in § 2 that (1.1) can be reduced to the study of the following far more tractable set of nonlinear ordinary differential equations:

$$
\begin{aligned}
\frac{dx_1}{dt} &= -x_1 - \beta(x_1 - T_c) + DBf(x_1, x_2), \\
\frac{dx_2}{dt} &= -x_2 + Df(x_1, x_2), \\
x_1(0) &= \int_0^1 \phi(\xi)\, d\xi, \\
x_2(0) &= \int_0^1 \psi(\xi)\, d\xi.
\end{aligned}
\tag{1.3}
$$

Here x_1 is the dimensionless temperature, and x_2 is the dimensionless concentration. These equations (1.3) are precisely the equations governing the enthalpy and mass balance for a single exothermic reaction occurring in a continuous stirred tank reactor [3].

In the chemical engineering literature the correspondence between (1.1) and (1.3) has been established *in the limit as the Peclet number $P \to 0$* by a technique called lumping (see Hlavacek and Hofmann [4] and McGowin and Perlmutter [7] and their references). We show that (1.3) is a valid approximation in a much wider sense. More precisely, when the first approximation equation of a certain expansion procedure covers a sufficiently broad class of problems, it is often adopted as an *approximate equation* for that class of problems, such as the transonic equation or the water wave equation. We shall show that the equations (1.3) are the first approximation in a self-consistent singular perturbation expansion procedure applied to problem (1.1) for small Peclet number (i.e., $0 < P \ll 1$), and therefore, the equations (1.3) are, in fact, valid approximate equations describing highly diffusive (or small Peclet number) reactions in the tubular reactor. Furthermore, just as in the transonic airfoil approximation or the water wave equation the accuracy of the approximation (or approximating equation) is known from the next term in the perturbation expansion. (See Cole [2, Chap. 5] for a further discussion of approximate field equations.)

An extensive treatment of the problem (1.3) is contained in the recent work of A. B. Poore [8], who has accounted for all possible situations which can occur in the continuous stirred tank reactor. These results coupled with our establishment in § 2 of (1.3) as the correct approximate equations for all small Peclet number tubular reactors will then imply the same exhaustive results for small Peclet number tubular reactors.

In § 3 we shall focus our attention on a few interesting newly discovered types of phenomena involving multiplicity, stability and bifurcation of periodic solutions and steady states. In particular, by means of numerical calculations and phase plane illustrations we follow the bifurcated periodic solution branches along their complete lengths.

2. The approximate equations. In this section we shall utilize an appropriate singular perturbation procedure which will establish the continuous stirred tank reactor equations (1.3) as the proper approximate equations for small Peclet number (or highly diffusive) turbular reactors.

Assume that $0 < P \ll 1$. We now construct the asymptotic expansions of the solutions of (1.1) as $P \to 0$. In this case we find by the techniques of singular perturbation theory [2] that there is an initial boundary layer of thickness $O(P)$ near $t = 0$ for all x in $0 \leqq x \leqq 1$. Away from this boundary layer the form of the asymptotic expansion (the outer solution) is given by

$$T(x,t) \sim \sum_{n=0}^{\infty} T_n(x,t)P^n, \qquad C(x,t) \sim \sum_{n=0}^{\infty} C_n(x,t)P^n. \tag{2.1}$$

Inserting (2.1) into (1.1) and equating coefficients of like powers of P, we find that to order P^2 we obtain

$$\begin{aligned} &\frac{\partial^2 T_0}{\partial x^2} = 0, && \frac{\partial^2 C_0}{\partial x^2} = 0, \\ &\frac{\partial T_0}{\partial x}(0,t) = 0, && \frac{\partial C_0}{\partial x}(0,t) = 0, \\ &\frac{\partial T_0}{\partial x}(1,t) = 0, && \frac{\partial C_0}{\partial x}(1,t) = 0, \end{aligned} \tag{2.2}$$

$$\begin{aligned} &\frac{\partial^2 T_1}{\partial x^2} = \frac{\partial T_0}{\partial t} + \frac{\partial T_0}{\partial x} + \beta(T_0 - T_c) - DB(1 - C_0)\exp\left(\frac{T_0}{1+\varepsilon T_0}\right), \\ &\frac{\partial^2 C_1}{\partial x^2} = \frac{\partial C_0}{\partial t} + \frac{\partial C_0}{\partial x} - D(1 - C_0)\exp\left(\frac{T_0}{1+\varepsilon T_0}\right), \\ &\frac{\partial T_1}{\partial x}(0,t) = T_0(0,t), \qquad \frac{\partial C_1}{\partial x}(0,t) = C_0(0,t), \\ &\frac{\partial T_1}{\partial x}(1,t) = 0, \qquad \frac{\partial C_1}{\partial x}(1,t) = 0. \end{aligned} \tag{2.3}$$

Equations (2.2) imply that

$$T_0(x,t) = x_1(t), \qquad C_0(x,t) = x_2(t), \tag{2.4}$$

where at this stage $x_1(t)$ and $x_2(t)$ are arbitrary functions of time. In order to determine them we must proceed to the next step in the perturbation procedure. Using (2.4), we can write the differential equations in (2.3) as

$$\tag{2.5} \begin{aligned} \frac{\partial^2 T_1}{\partial x^2} &= \frac{dx_1}{dt} + \beta(x_1 - T_c) - DB(1 - x_2)\exp\left(\frac{x_1}{1 + \varepsilon x_1}\right) \equiv A(t), \\ \frac{\partial^2 C_1}{\partial x^2} &= \frac{dx_2}{dt} - D(1 - x_2)\exp\left(\frac{x_1}{1 + \varepsilon x_1}\right) \equiv B(t). \end{aligned}$$

Thus, $T_1(x, t) = \frac{1}{2}A(t)x^2 + c_1(t)x + c_2(t)$ and $C_1(x, t) = \frac{1}{2}B(t)x^2 + c_3(t)x + c_4(t)$, where the $c_i(t)$, $i = 1, \cdots, 4$, are arbitrary functions. The boundary conditions at $x = 0$ in (2.3) imply that $c_1(t) = x_1(t)$ and $c_3(t) = x_2(t)$. Finally, to satisfy the boundary conditions at $x = 1$ in (2.3) we find that we must have $A(t) + x_1(t) = 0$ and $B(t) + x_2(t) = 0$; that is, we must have

$$\tag{2.6} \begin{aligned} \frac{dx_1}{dt} &= -x_1 - \beta(x_1 - T_c) + DB(1 - x_2)\exp\left(\frac{x_1}{1 + \varepsilon x_1}\right), \\ \frac{dx_2}{dt} &= -x_2 + D(1 - x_2)\exp\left(\frac{x_1}{1 + \varepsilon x_1}\right). \end{aligned}$$

Thus, the functions $x_1(t)$ and $x_2(t)$ are determined from compatibility conditions (2.6) which they must satisfy in order to generate a consistent perturbation procedure. (An alternative and more elegant way to obtain (2.6) is to recognize that equations (2.3) constitute an inhomogeneous form of (2.2) and use a version of the Fredholm alternative theorem. In the present case this amounts to integrating the equations in (2.3) with respect to x from 0 to 1 and using the boundary conditions.)

We now obtain the appropriate initial conditions for $x_1(t)$ and $x_2(t)$ by a matching procedure with the asymptotic form in the initial boundary layer. Set $\tau = t/P$, and let $T(x, t) = T(x, P\tau) \equiv \tilde{T}(x, \tau)$, $C(x, t) = C(x, P\tau) \equiv \tilde{C}(x, \tau)$. Then, (1.1) becomes

$$\tag{2.7} \begin{aligned} &\frac{\partial \tilde{T}}{\partial \tau} - \frac{\partial^2 \tilde{T}}{\partial x^2} = P\left[-\frac{\partial \tilde{T}}{\partial x} - \beta(\tilde{T} - T_c) + DB(1 - \tilde{C})\exp\left(\frac{\tilde{T}}{1 + \varepsilon\tilde{T}}\right)\right], \\ &\frac{\partial \tilde{C}}{\partial \tau} - \frac{\partial^2 \tilde{C}}{\partial x^2} = P\left[-\frac{\partial \tilde{C}}{\partial x} + D(1 - \tilde{C})\exp\left(\frac{\tilde{T}}{1 + \varepsilon\tilde{T}}\right)\right], \\ &\frac{\partial \tilde{T}}{\partial x}(0, \tau) = P\tilde{T}(0, \tau), \qquad \frac{\partial \tilde{C}}{\partial x}(0, \tau) = P\tilde{C}(0, \tau), \\ &\frac{\partial \tilde{T}}{\partial x}(1, \tau) = 0, \qquad \frac{\partial \tilde{C}}{\partial x}(1, \tau) = 0, \\ &\tilde{T}(x, 0) = \phi(x), \qquad \tilde{C}(x, 0) = \psi(x). \end{aligned}$$

The asymptotic expansion (the main solution) in the initial layer is given by

$$\tag{2.8} \tilde{T}(x, \tau) \sim \sum_{n=0}^{\infty} \tilde{T}_n(x, \tau)P^n, \qquad \tilde{C}(x, \tau) \sim \sum_{n=0}^{\infty} \tilde{C}_n(x, \tau)P^n.$$

Upon substituting (2.8) into (2.7), we find that to first order in P we obtain

$$
\begin{aligned}
&\frac{\partial^2 \tilde{T}_0}{\partial \tau} = \frac{\partial^2 \tilde{T}_0}{\partial x^2}, && \frac{\partial^2 \tilde{C}_0}{\partial \tau} = \frac{\partial^2 \tilde{C}_0}{\partial x^2},\\
&\frac{\partial \tilde{T}_0}{\partial x}(0, \tau) = 0, && \frac{\partial \tilde{C}_0}{\partial x}(0, \tau) = 0,\\
&\frac{\partial \tilde{T}_0}{\partial x}(1, \tau) = 0, && \frac{\partial \tilde{C}_0}{\partial x}(1, \tau) = 0,\\
&\tilde{T}_0(x, 0) = \phi(x), && \tilde{C}_0(x, 0) = \psi(x).
\end{aligned}
\tag{2.9}
$$

Therefore,

$$
\begin{aligned}
\tilde{T}_0(x, \tau) &= A_0 + \sum_{n=1}^{\infty} A_n e^{-n^2\pi^2\tau} \cos n\pi x,\\
\tilde{C}_0(x, \tau) &= B_0 + \sum_{n=1}^{\infty} B_n e^{-n^2\pi^2\tau} \cos n\pi x,
\end{aligned}
\tag{2.10}
$$

where

$$
\begin{aligned}
A_0 &= \int_0^1 \phi(\xi)\, d\xi, \qquad & A_n &= 2\int_0^1 \phi(\xi) \cos n\pi\xi \, d\xi,\\
B_0 &= \int_0^1 \psi(\xi)\, d\xi, \qquad & B_n &= 2\int_0^1 \psi(\xi) \cos n\pi\xi \, d\xi.
\end{aligned}
\tag{2.11}
$$

Equations (2.10), (2.11) give the first term (i.e., the zero order term) in the asymptotic expansion of the solution (the inner solution) of (1.1) in the initial boundary layer. The standard matching of inner and outer solutions now requires that

$$
\begin{aligned}
\lim_{t \to \infty} [T_0(x, t)] &= \lim_{\tau \to \infty} [\tilde{T}_0(x, \tau)],\\
\lim_{t \to 0} [C_0(x, t)] &= \lim_{\tau \to \infty} [\tilde{C}_0(x, \tau)].
\end{aligned}
$$

Thus, $x_1(0) = A_0$ and $x_2(0) = B_0$, and the equations governing $x_1(t)$ and $x_2(t)$ are

$$
\begin{aligned}
\frac{dx_1}{dt} &= -x_1 - \beta(x_1 - T_c) + DB(1 - x_2) \exp\left(\frac{x_1}{1 + \varepsilon x_1}\right),\\
\frac{dx_2}{dt} &= -x_2 + D(1 - x_2) \exp\left(\frac{x_1}{1 + \varepsilon x_1}\right),\\
x_1(0) &= A_0 = \int_0^1 \phi(\xi)\, d\xi,\\
x_2(0) &= B_0 = \int_0^1 \psi(\xi)\, d\xi.
\end{aligned}
\tag{2.12}
$$

Therefore, subtracting the part of the expansion common to both inner and outer expansions [2] we obtain the following asymptotic expansions as $P \to 0$ of the solution of (1.1) which is *uniformly valid* on $t \geqq 0, 0 \leqq x \leqq 1$:

$$\text{(2.13)} \quad \begin{aligned} T(x,t) &= x_1(t) + \sum_{n=1}^{\infty} A_n \exp\left\{-n^2\pi^2 \frac{t}{P}\right\} \cos n\pi x + O(P), \\ C(x,t) &= x_2(t) + \sum_{n=1}^{\infty} B_n \exp\left\{-n^2\pi^2 \frac{t}{P}\right\} \cos n\pi x + O(P), \end{aligned}$$

where $x_1(t)$ and $x_2(t)$ satisfy (2.12) and A_n and B_n are given by (2.11). Note that in the usual way the entire infinite sums in (2.13) are negligible compared with $x_1(t)$ and $x_2(t)$ outside the initial boundary layer, and thus, after a short initial time during which standard linear diffusion governs the process, the solution to $O(P)$ is basically $T(x, t) \sim x_1(t), C(x, t) \sim x_2(t)$.

Higher order correction terms can clearly be found by continuing our procedure in the same way. For example, with $x_1(t)$ and $x_2(t)$ chosen to satisfy (2.12) the solution of (2.3) is given by

$$\begin{aligned} T_1(x,t) &= -\tfrac{1}{2}(x-1)^2 x_1(t) + x_3(t), \\ C_1(x,t) &= -\tfrac{1}{2}(x-1)^2 x_2(t) + x_4(t), \end{aligned}$$

where $x_3(t)$ and $x_4(t)$ are arbitrary functions of time which can be determined from a compatibility condition necessary in the next step of the perturbation procedure.

3. Bifurcation of oscillatory states. We shall now examine some interesting cases of bifurcation of periodic orbits as the Damkohler number D passes through certain critical values. For algebraic simplicity we set $\varepsilon = 0$ in problem (2.6) and consider

$$\text{(3.1)} \quad \begin{aligned} \frac{dx_1}{dt} &= -x_1 - \beta(x_1 - T_c) + DB(1 - x_2)\, e^{x_1} \equiv F_1(\mathbf{x}), \\ \frac{dx_2}{dt} &= -x_2 + D(1 - x_2)\, e^{x_1} \equiv F_2(\mathbf{x}). \end{aligned}$$

Let

$$m_1 = \frac{1}{2} - \frac{1}{2}\sqrt{1 - \frac{4(1+\beta)}{B}}, \qquad m_2 = \frac{1}{2} + \frac{1}{2}\sqrt{1 - \frac{4(1+\beta)}{B}},$$

$$s_1 = \frac{B+1+\beta}{2} - \frac{1}{2B}\sqrt{(B+1+\beta)^2 - 2B(2+\beta)},$$

$$s_2 = \frac{B+1+\beta}{2} + \frac{1}{2B}\sqrt{(B+1+\beta)^2 - 2B(2+\beta)},$$

and define D_i $(i = 1, \cdots, 4)$ by $D_1 = D(m_1)$, $D_2 = D(m_2)$, $D_3 = D(s_1)$, $d_4 = D(s_2)$, where

$$D(\tau) = \frac{\tau}{1-\tau} \exp\left(\frac{-B\tau}{1+\beta} - \frac{\beta T_c}{1+\beta}\right).$$

The point

$$\mathbf{a}^0 = \left(\frac{Bs_i}{1+\beta} - \frac{\beta T_c}{1+\beta}, s_i\right) \tag{3.2}$$

is a critical point of (3.1), and this critical point is a center for the linearized problem about $\mathbf{a}^0$ whenever $B > 4(1+\beta)$, $B > 3 + \beta + 2\sqrt{2+\beta}$, $s_i \in (0, m_1) \cup (m_2, 1)$, $i = 1, 2$, or whenever $3 + \beta + 2\sqrt{2+\beta} < B < 4(1+\beta)$. (The calculations supporting this fact are given in [8]. Also see Figs. 1–8.)

Bifurcation of oscillatory states in our system comes about essentially in the following way: As the Damkohler number D varies, a critical point of (3.1) changes from a stable spiral point of the linearized system to an unstable spiral point. At the point of change, the spiral point becomes a center, the value of D at this point is the critical Damkohler number D_0, and a bifurcation of an oscillatory state ensues. To make this precise we shall need the Friedrichs bifurcation theorem [10, p. 122]. This necessitates the introduction of the following notation:

$$\begin{aligned} &D = D_0 + \varepsilon, \quad \mathbf{a}^\varepsilon = \mathbf{a}(D_0 + \varepsilon), \quad s = (T^0/T^\varepsilon)t, \quad \varepsilon = \mu\delta, \\ &T^\varepsilon = T^0(1 + \mu\eta), \quad \mathbf{x}^\varepsilon = \mathbf{a}^\varepsilon + \mu\mathbf{y}(s, \mu), \quad A^\varepsilon = \mathbf{F}_x(\mathbf{a}^\varepsilon, \varepsilon), \\ &\varepsilon C^\varepsilon = A^\varepsilon - A^0, \qquad C^0 = \left.\frac{dA^\varepsilon}{d\varepsilon}\right|_{\varepsilon=0}, \\ &\mu^2 Q^\varepsilon(\mathbf{y}, \mu) = \mathbf{F}(\mathbf{a}^\varepsilon + \mu\mathbf{y}, \varepsilon) - \mu A^\varepsilon \mathbf{y}, \end{aligned} \tag{3.3}$$

where

$$T^0 = \sqrt{\det(\mathbf{F}_x(\mathbf{a}^0, 0))},$$

$\mathbf{a}^0$ is given by (3.2), and η and δ are two parameters to be determined. We have written the critical point $\mathbf{a}^\varepsilon$ as a function of ε; i.e., $\mathbf{a}^\varepsilon = \mathbf{a}(D_0 + \varepsilon)$. That this is valid follows from the fact that $\mathbf{a}^0$ is a center for linearized problems which implies that $\det \mathbf{F}_x(\mathbf{a}^0, 0) \neq 0$, so that the implicit function theorem yields the desired fact. Under the change of variables (3.3), system (3.1) becomes

$$\frac{d\mathbf{y}}{ds} = A^0\mathbf{y} + \mu\{\delta C^\varepsilon \mathbf{y} + \eta A^\varepsilon \mathbf{y} + (1 + \mu\eta)Q^\varepsilon(\mathbf{y}, \mu)\}, \tag{3.4}$$

where

$$A^\varepsilon = \begin{pmatrix} Ba_2^\varepsilon - 1 - \beta & -Ba_2^\varepsilon/(1 - a_2^\varepsilon) \\ a_2^\varepsilon & -1/(1 - a_2^\varepsilon) \end{pmatrix},$$

$$C^0 = \begin{pmatrix} B & -1/(1 - a_2^0) \\ 1 & -1/(1 - a_2^0)^2 \end{pmatrix} \left.\frac{da_2^\varepsilon}{d\varepsilon}\right|_{\varepsilon=0},$$

$$Q^\varepsilon(\mathbf{y}, \mu) = \frac{a_2^\varepsilon}{1 - a_2^\varepsilon} \left\{ \begin{matrix} B\left\{\dfrac{1 - a_2^\varepsilon}{\mu^2}(e^{\mu y_1} - 1 - \mu y_1) - \dfrac{y_2}{\mu}(e^{\mu y_1} - 1)\right\} \\ \left\{\dfrac{1 - a_2^\varepsilon}{\mu^2}(e^{\mu y_1} - 1 - \mu y_1) - \dfrac{y_2}{\mu}(e^{\mu y_1} - 1)\right\} \end{matrix} \right\}.$$

Friedrichs' bifurcation theorem now implies the following theorem.

THEOREM 3.1. *Let β, B and D_0 be chosen as above so that $\mathbf{a}^0$ is a center for the linearized problem associated with* (3.1). *Then, there exist functions $\eta = \eta(\mu)$ and $\delta = \delta(\mu)$ with $\varepsilon = \mu\delta(\mu)$, $T^\varepsilon = T^0(1 + \mu\eta(\mu))$, $\delta(0) = \eta(0) = 0$, and $\delta(\mu)$, $\eta(\mu) \in C'(-\mu_0, \mu_0)$ for some sufficiently small $\mu_0 > 0$ and a function $\mathbf{y}(s, \mu)$ with period T^0 in s assuming an arbitrarily prescribed initial value $\mathbf{y}(0, \mu) = \mathbf{b}_0$ such that*

$$\mathbf{x}^\varepsilon = \mathbf{a}^\varepsilon + \mu\mathbf{y}(s, \mu) \tag{3.5}$$

is a solution of the differential equation (3.1).

Since $D - D_0 = \varepsilon = \mu\delta(\mu)$, $\delta(0) = 0$, $\delta \in C'(-\mu_0, \mu_0)$, it follows that $D = D_0 + \mu^2\delta'(0) + O(\mu^2)$. Thus, the sign of $\delta'(0)$ determines the direction of bifurcation in the sense that the bifurcated periodic solution in (3.5) surrounds the critical point $\mathbf{a}(D)$, where $D > D_0$ ($<D_0$) for $\delta'(0) > 0$ (<0) and D close to D_0. The $\delta'(0)$ comes from a periodicity condition in the proof of Theorem 3.1 as in [8] or [9]. More explicitly, $\delta'(0)$ and $\eta'(0)$ satisfy

$$\begin{aligned} &\eta'(0)\int_0^{T^0} \mathbf{Y}^{-1}(s)A^0\mathbf{y}(s,0)\,ds + \delta'(0)\int_0^{T^0} \mathbf{Y}^{-1}(s)C^0\mathbf{y}(s,0)\,ds \\ &\quad = -\int_0^{T^0} Y^{-1}(s)\left(\frac{dQ^\varepsilon}{d\mu}(\mathbf{y}(s,\mu),\mu)\right)\bigg|_{\mu=0} ds. \end{aligned} \tag{3.6}$$

By solving this sytem of equations one can show that

$$\delta'(0) = \frac{Ba^2b^2}{8\omega_0^4 \operatorname{tr} C_0}\{\omega_0^2(b - 1) + (2b - Ba) - (2b - Ba)^2\}, \tag{3.7}$$

where $b = Bs_i - 1 - \beta$, $a = s_i$, $\omega_0^2 = \det A^0 = Ba^2b - b^2$.

The stability of the bifurcated periodic orbits can be established by using Poincaré's criterion. Namely, if $\mathbf{H}(\mathbf{y}(s, \mu), \mu)$ denotes the right-hand side of (3.4), then by expanding $\nabla \cdot \mathbf{H}(\mathbf{y}, \mu)$ in powers of μ it follows that

$$\int_0^{T^0} \nabla \cdot \mathbf{H}(\mathbf{y}(s,\mu),\mu)\,ds = -(\operatorname{tr} C^0)\delta'(0)\mu^2 + O(\mu^2) \quad \text{as } \mu \to 0, \tag{3.8}$$

where the divergence is with respect to $\mathbf{y}$. Thus from Poincaré's criterion (see W. A. Coppel [10]), we can conclude that $\int_0^{T^0} \nabla \cdot \mathbf{H}(\mathbf{y}, \mu)\,ds < 0$ (>0) if $-(\operatorname{tr} C^0)\delta'(0) < 0$ (>0) for μ sufficiently small (and thus D close to D_3 or D_4) so that the periodic orbit is asymptotically orbitally stable if $-(\operatorname{tr} C^0)\delta'(0) < 0$ and is unstable if $-(\operatorname{tr} C^0)\delta'(0) > 0$. Algebraic manipulations show that $\operatorname{tr} C^0 < 0$ (>0) for $D = D_3$,

$$\mathbf{a}^0 = \left(\frac{Bs_1}{1+\beta}s_1 - \frac{\beta P_c}{1+\beta}, s_1\right) \quad \left(D = D_4, \quad \mathbf{a}^0 = \left(\frac{Bs_2}{1+\beta}s_2 - \frac{\beta T_c}{1+\beta}, s_2\right)\right).$$

To illustrate these results we now describe several interesting situations which are illustrated in Figs. 1–8. For Figs. 1 and 2 we have taken $T_c = 0$, $\beta = 3.0$, and $B = 14.0$. For these parameter values, there is a unique critical point of (3.1) for all $D > 0$. The critical point is asymptotically stable when

$$D \in (0, D_3) \cup (D_4, \infty) = (0, 0.1650) \cup (0.3366, \infty)$$

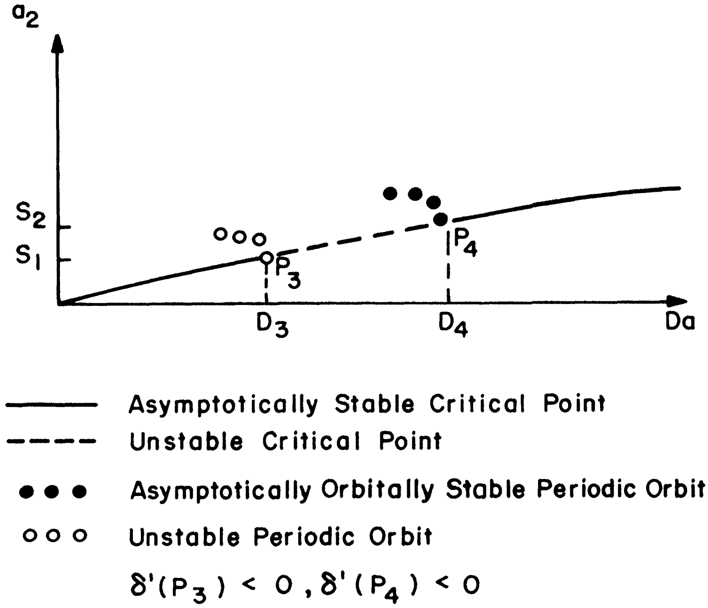

a2
S2
S1
P3
P4
D3
D4
Da
Asymptotically Stable Critical Point
Unstable Critical Point
Asymptotically Orbitally Stable Periodic Orbit
Unstable Periodic Orbit
δ'(P3) < 0 , δ'(P4) < 0

FIG. 1

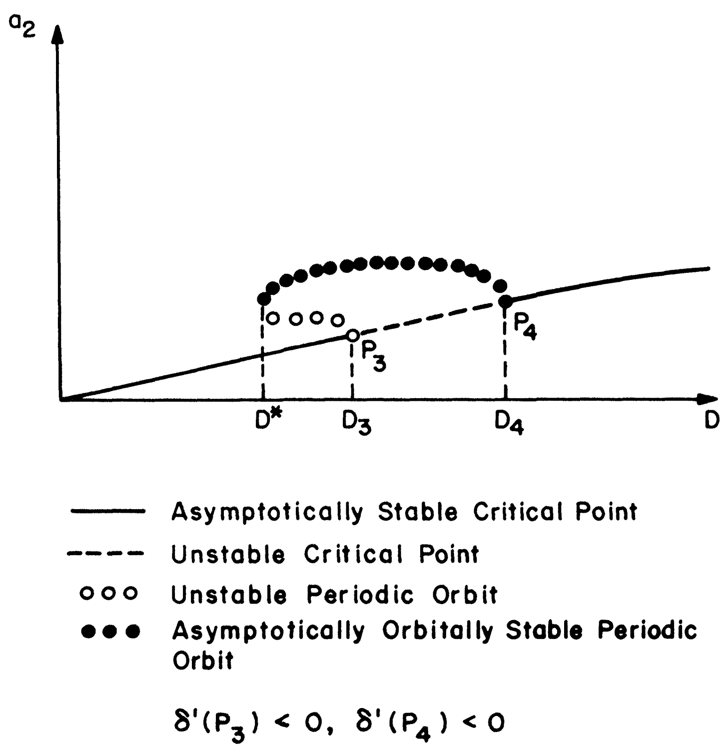
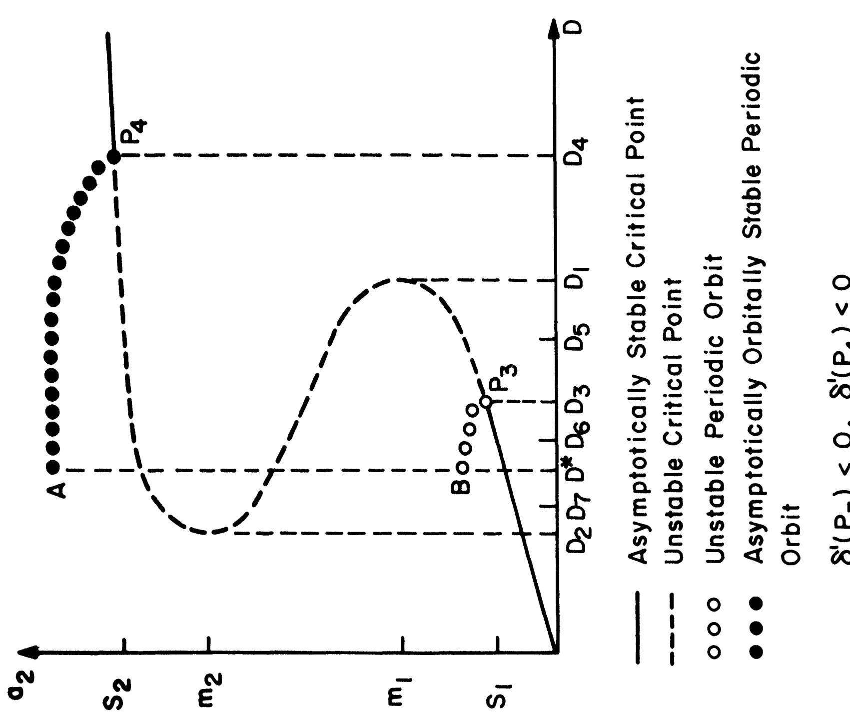
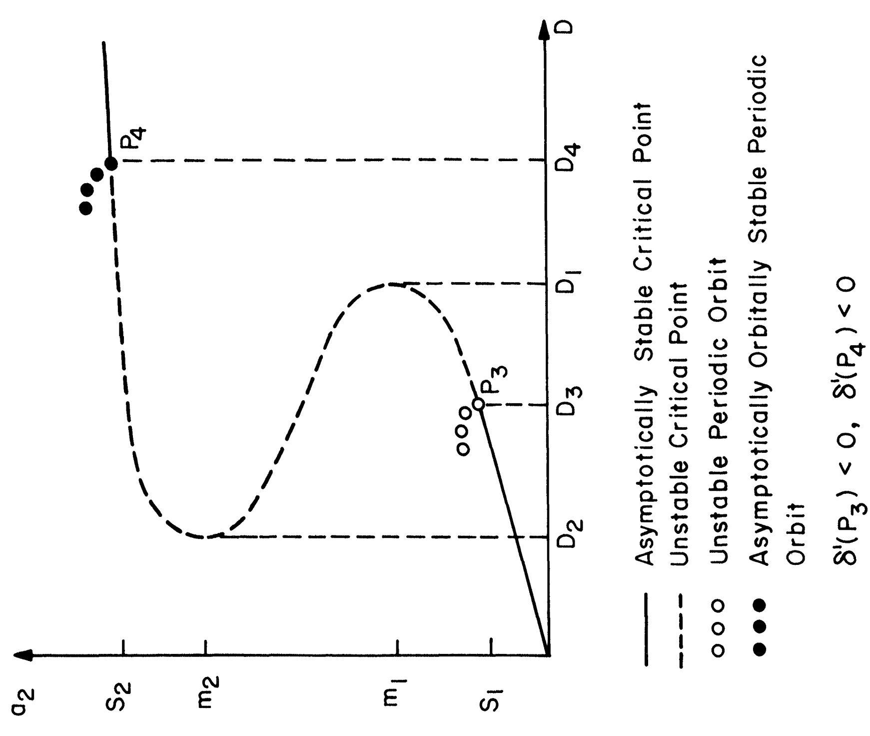

a2
P3
P4
D*
D3
D4
D
Asymptotically Stable Critical Point
Unstable Critical Point
Unstable Periodic Orbit
Asymptotically Orbitally Stable Periodic Orbit
δ'(P3) < 0, δ'(P4) < 0

FIG. 2



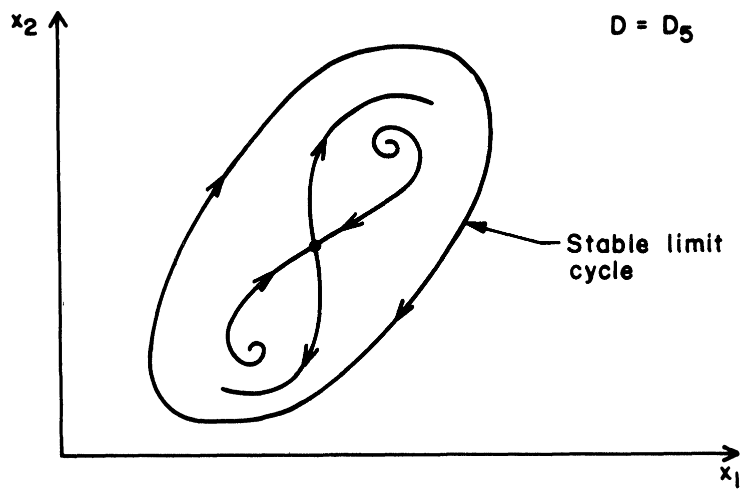
a_2
s_2
m_2
m_1
s_1
D
P_4
A
B
P_3
D_2 D_7 D^* D_6 D_3 D_5 D_1 D_4
Asymptotically Stable Critical Point
Unstable Critical Point
Unstable Periodic Orbit
Asymptotically Orbitally Stable Periodic Orbit
$\delta'(P_3) < 0, \ \delta'(P_4) < 0$

FIG. 4



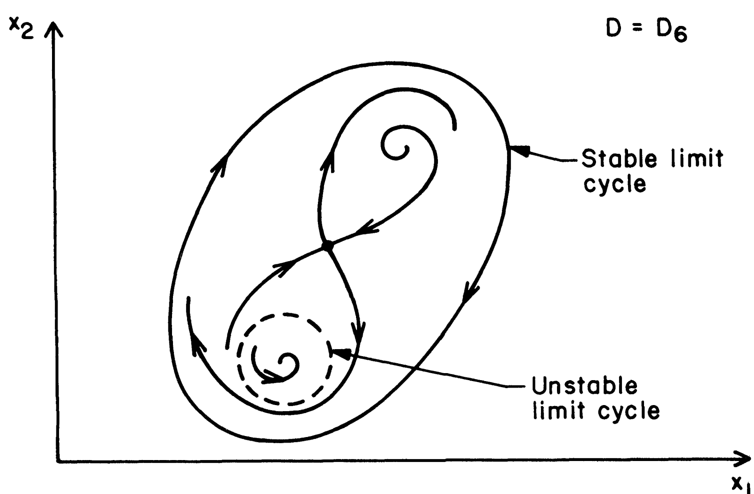
a_2
s_2
m_2
m_1
s_1
D
P_4
P_3
D_2 D_3 D_1 D_4
Asymptotically Stable Critical Point
Unstable Critical Point
Unstable Periodic Orbit
Asymptotically Orbitally Stable Periodic Orbit
$\delta'(P_3) < 0, \ \delta'(P_4) < 0$

FIG. 3



x_2
$D = D_5$
Stable limit cycle
x_1

FIG. 5



x_2
$D = D_6$
Stable limit cycle
Unstable limit cycle
x_1

FIG. 6

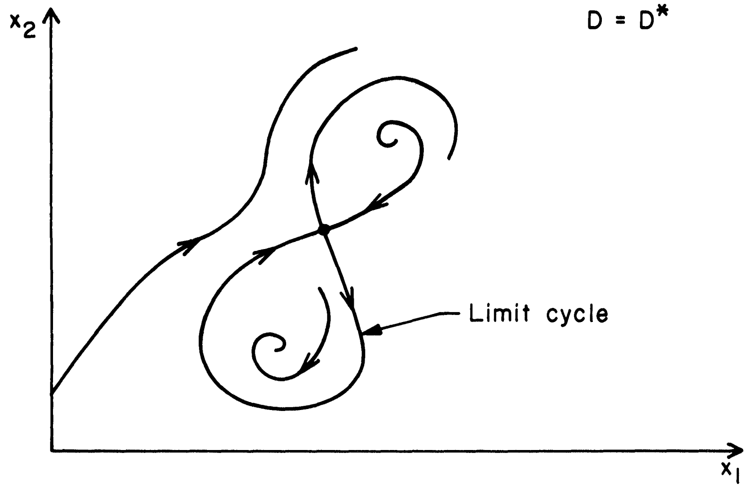


FIG. 7

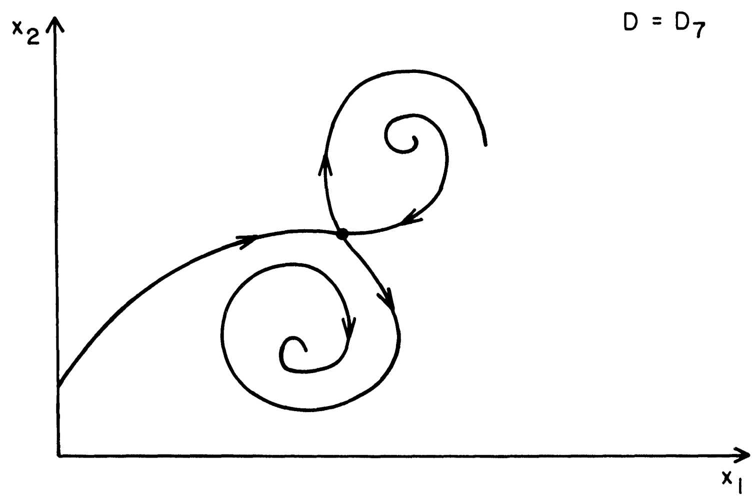


FIG. 8

and is unstable when

$$D \in (D_3, D_4) = (0.1650, 0.3366).$$

The critical point $\mathbf{a}^0 = (Bs_i/(1 + \beta), s_i)$ is a center for the linearized problem so that Theorem 3.1 applies. By numerically evaluating $\delta'(0)$, one can show that $\delta'(0) < 0$ for $i = 1$ and 2. Theorem 3.1 states that for D less than but close to D_3 or D_4 there is a periodic orbit whose diameter goes to zero as $D \to D_3$ or D_4.

Thus, in Fig. 1, the vertical distance between the periodic orbit and the critical point denotes the maximum deviation of the periodic orbit from the critical point. At the point $P_4 = (Bs_2/(1 + \beta), s_2)$ we have $\operatorname{tr} C^0 > 0$ so that the integral in (3.8) is negative for μ sufficiently small (since $\delta'(0) < 0$ also holds at P_4). Thus, the periodic orbit bifurcating to the left at D_4 is asymptotically orbitally stable. Next, $\operatorname{tr} C^0 < 0$ and $\delta'(0) < 0$ at the point $P_4 = (Bs_1/(1 + \beta), s_1)$ so the integral in (3.8) is positive for μ sufficiently small which implies that the bifurcated periodic orbits from D_3 are unstable (D close to D_3). Since the applicability of the Poincaré–Bendixson theory to this problem has been established (see [8]), there must exist at least one periodic orbit for each $D \in (D_3, D_4)$; furthermore, there exists at least one more periodic orbit surrounding the unstable periodic orbit corresponding to D close to but less than D_3. Actual numerical computations [11] show that the branch of periodic solutions is continued as in Fig. 2.

A more interesting case occurs when there are multiple critical points and bifurcation phenomena. Such a case occurs when we choose $T_c = 0$, $\beta = 3.0$, $B = 19.0$, and is illustrated in Figs. 3–8. There is exactly one critical point for $D \in (D_2, D_1)$. Theorem 3.1 is applicable, and a numerical evaluation shows that $\delta'(0) < 0$ at $P_3 = (Bs_1/(1 + \beta), s_1)$ and $P_4 = (Bs_2/(1 + \beta), s_2)$. Thus

$$-(\operatorname{tr} C^0)\delta'(0) > 0 \qquad (<0)$$

at P_3 (P_4). The bifurcated periodic orbits and their stability are indicated in Fig. 3 where again the vertical distance between the critical point and the periodic orbit denotes the maximum deviation of the periodic orbit from the critical point. We note that Theorem 3.1 is local in nature in that the branch of bifurcated periodic orbits is established for D sufficiently close to D_3 or D_4. For $D \in (D_1, D_4)$ the Poincaré–Bendixson theorem shows that there is a periodic orbit surrounding the unstable critical point for each D. For D close to but less than D_3 there is an unstable periodic orbit surrounding the stable point. The rest of Fig. 4 has been completed from numerical calculation [11] and the phase plane descriptions of Figs. 5–8. These need some careful discussion; we give this now.

Figure 4 is meant to imply that periodic orbits cease to exist at some $D = D^* \in (D_2, D_1)$. However, special care must be given to the interpretation of the periodic solution branches in Fig. 4. *Points A and B denote the same periodic solution.* To make this more explicit, consider the phase plane descriptions of Figs. 5–8 for the various values of D exhibited in Fig. 4. As D decreases from D_6 to D^*, the unstable limit cycle (the lower periodic branch of Fig. 4) grows until it coalesces with the stable limit cycle (the upper periodic branch of Fig. 4) near the bottom. Thus, at $D = D^*$ there exists one limit cycle (Fig. 7), and this is point A (the limit of the stable branch of oscillations as $D \to D^*$) or point B (the limit of the unstable branch of oscillations as $D \to D^*$). Perhaps, a more suggestive illustration would be to sketch a three-dimensional version of Fig. 4 in which the branches of periodic orbits are out of the plane of the paper. In this graph, then, we could join points A to point B, and as a norm near D^* we could use the maximum distance of the limit cycle from the unstable middle critical point (the saddle point). Clearly, then points A and B represent the situations of Fig. 7 at $D = D^*$.

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